Digital Designed Manufacturing of Precision Particulate Products (DigiP3)

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- **Aim**
  - Develop multi-scale modelling and characterisation tools (DigiP3) to digitally design & accurately manufacture precision particulate products for health (pharmaceutical), fine chemical, biotech etc. industries

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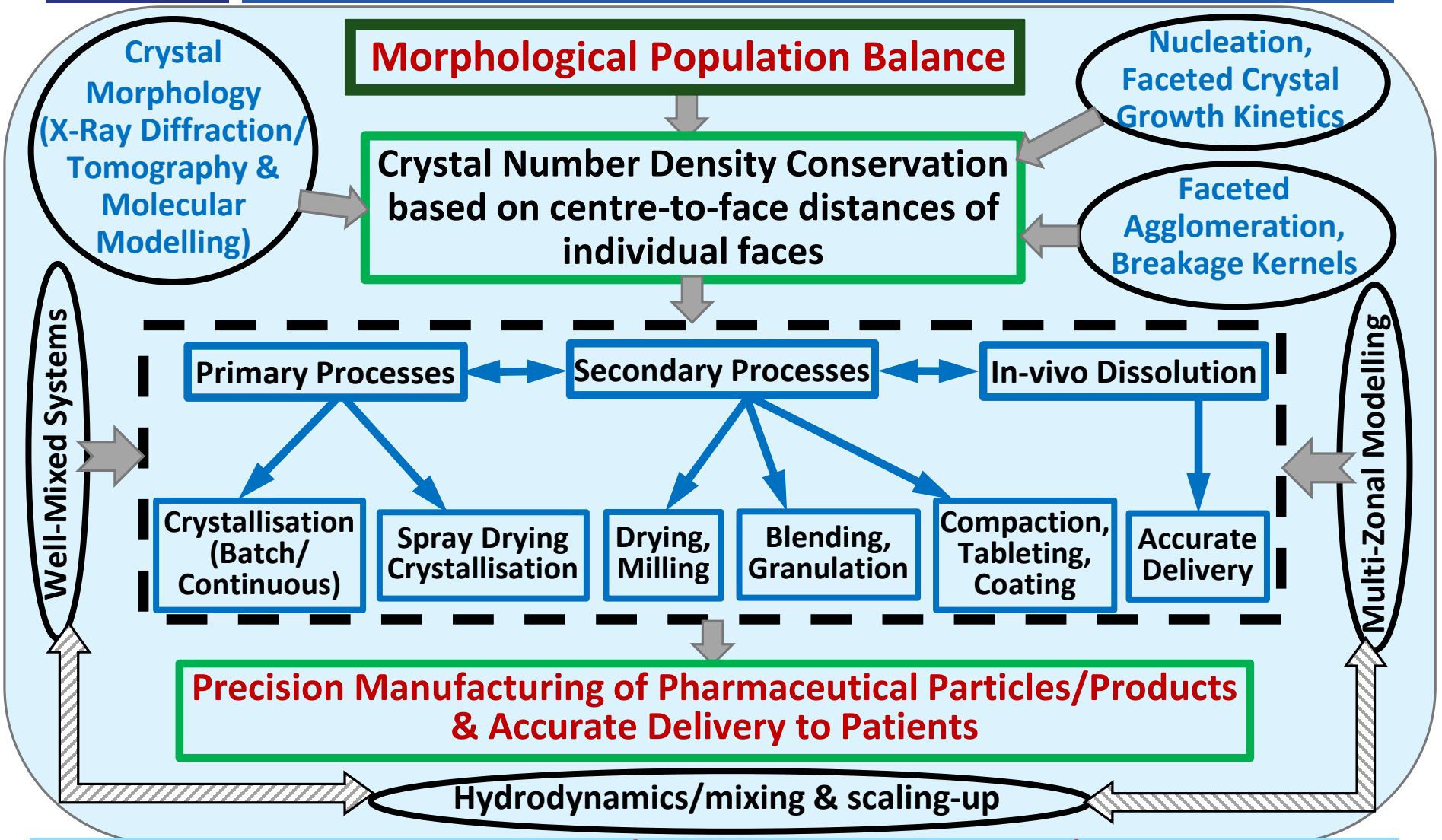
Precision Particle Design – A Morphological Approach



Importance & modelling of surface/liquid interface & surface/solution chemistry

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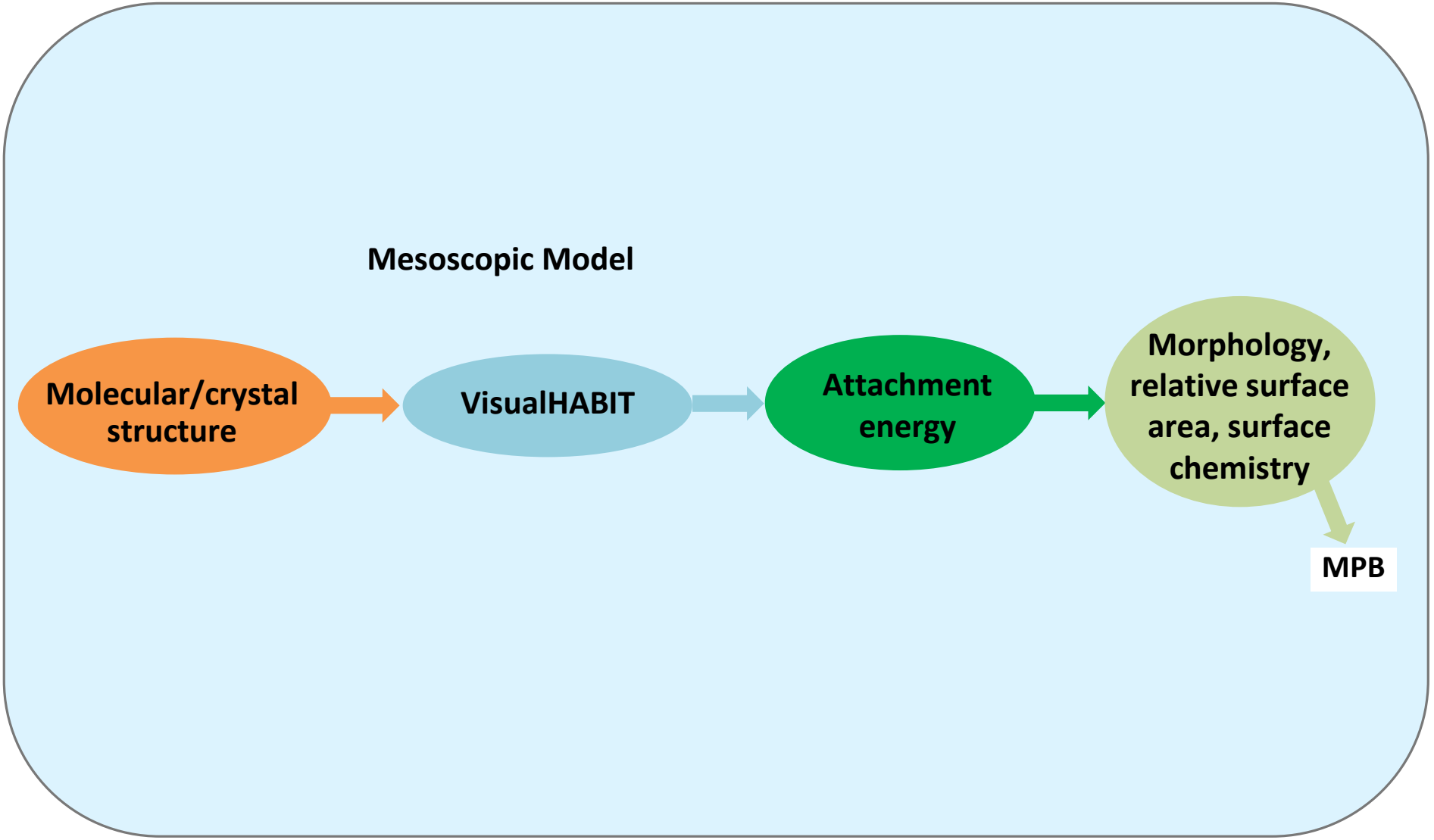
VisualHABIT



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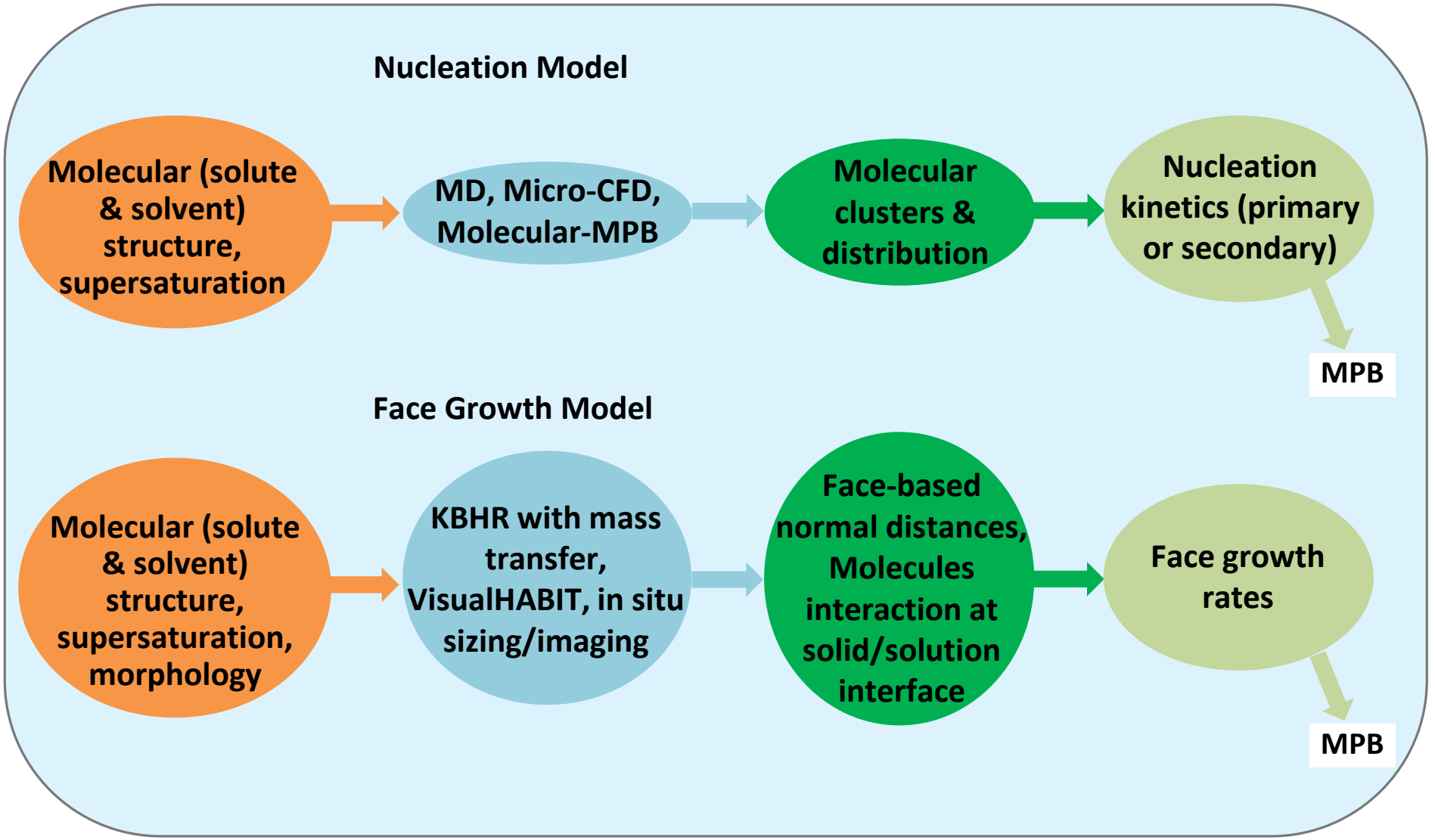
Nucleation & face growth kinetics



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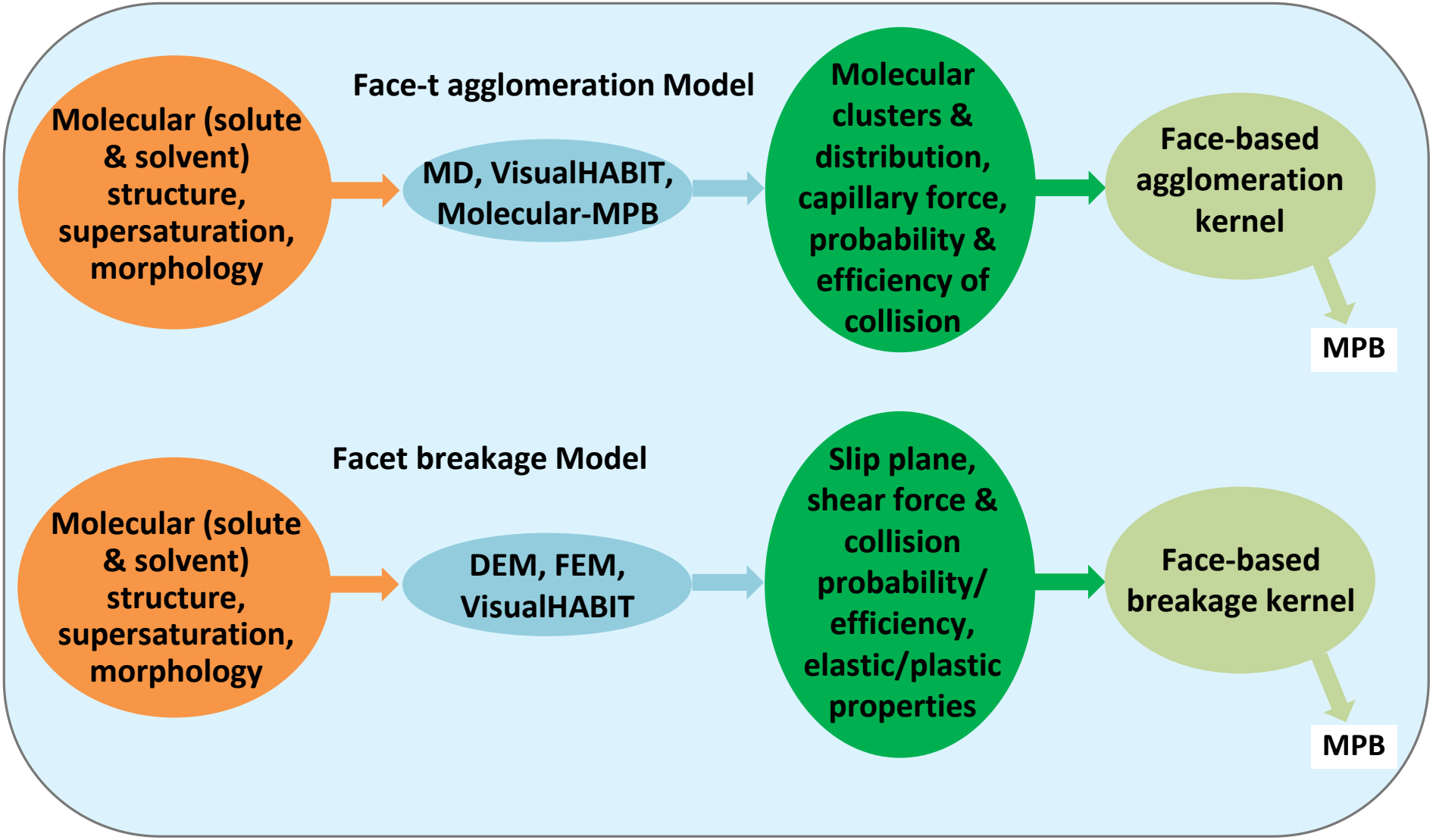
Face-based agglomeration & breakage kernels



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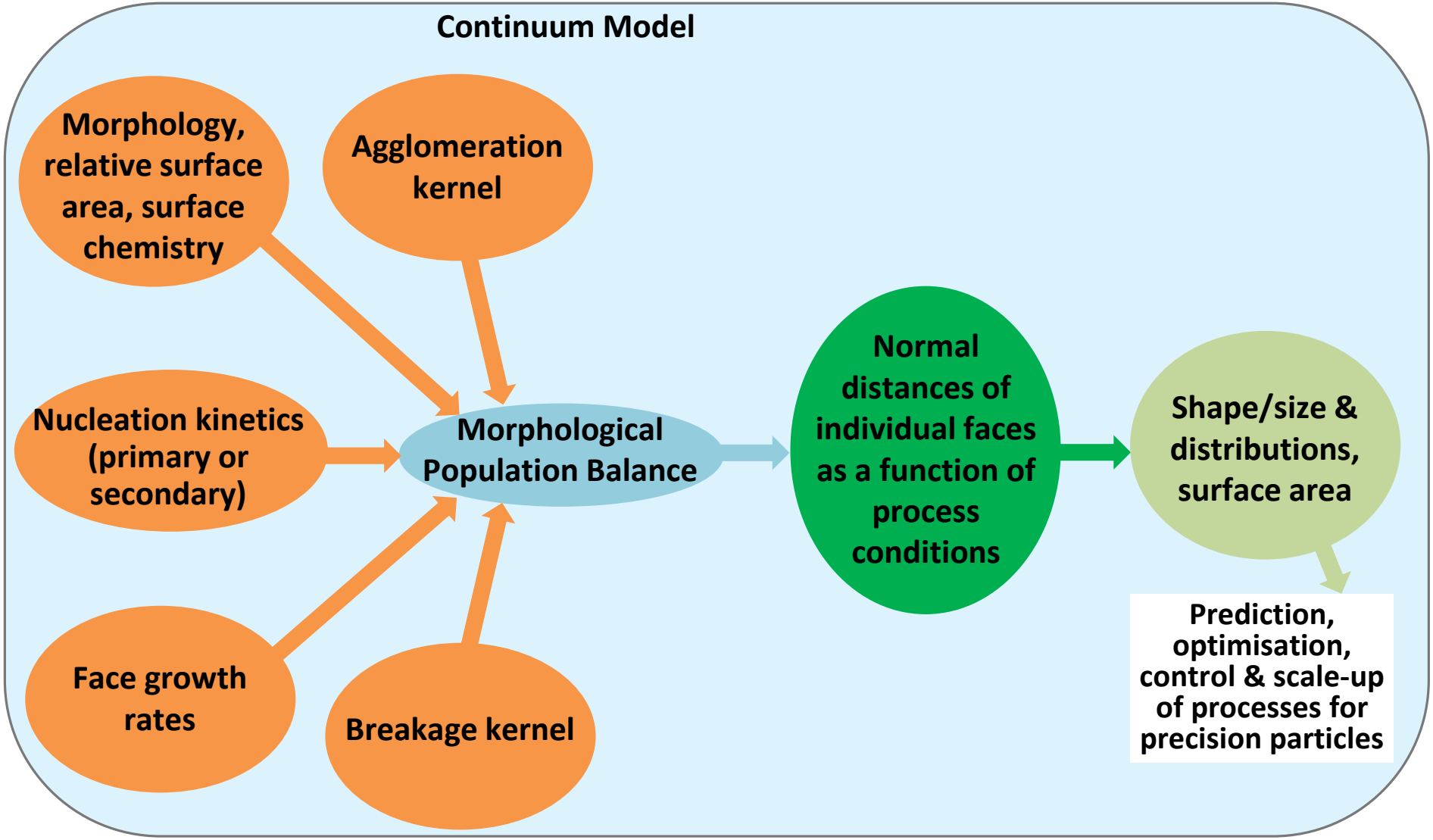
Morphological population balance



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DigiP3

- **Objectives**
  - To implement VisualHABIT/SystSearch (Leeds) into CCDC's Mercury for molecular/crystal (& morphological properties) modelling
  - To integrate kinetics at wetted surface/boundary/liquid bridge, facet growth kinetics, facet agglomeration & breakage kernels into MPB (morphological population balance) and their coupling with CFD
    - With MD & molecular-MPB, micro-CFD for molecular clusters, a molecular-based model accounting for wetted face, liquid bridge, shear-affected boundary for particulate processes involving in solid/solution interface
    - Facet growth mechanism, obtained from *in situ* growth measurement using particle sizing & imaging, for MPB model development & validation
    - Facet agglomeration & breakage with DEM/MD/molecular-MPB
  - To develop an integrated digital design platform (DigiP3) for precision manufacturing of particulate products
  - To enable particulate manufacturing companies to digitalise their processes for producing materials with highest added value

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DigiP3

- **Innovative Aspects**
  - Precision manufacturing of particles
  - Integrated models for digital design of pharmaceutical (& other particulate) manufacture processes
  - Mechanistic process models based on first-principles for wide range application of particle production and drug delivery

- **Expected Impact**
  - Significantly reduce experiments required by traditional try-and-error R&D mode
  - Speed up model blocks building for specific industrial process problems
  - Provide reliable working ranges and guides for decision making during precision manufacturing of particles

- **Expected Results**
  - A coupled micro-scale CFD, MPB & MD modelling framework for molecules/clusters behaviour at particle surface/solution boundary layer (TRL4)
  - First-principle mechanisms of 2nd nucleation & faceted growth kinetics, agglomeration/breakage kernels from coupled CFD-MPB-MD modelling (TRL4-5)
  - System-scale process model (DigiP3) for precision manufacturing of pharmaceuticals & other particulates (TRL4-6)
  - Case studies with industrial particle manufacturing systems (TRL4-6)

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- **Models identified (for development)**
  - Systematic search & VisualHABIT (Leeds)
  - Morphological population balance (Leeds)
  - Molecular dynamics (Hartree/Leeds)
  - CFD (OpenFoam, ANSYS) (Leeds/Hartree)
  - gPROMS Formulated Products (PSE)
  - Other models?
- **Partners**
  - Identified partners
    - TU Delft (Prof Herman Kramer)
    - Technobis (Stephan van Banning)
    - PSE (Sean Bermingham)
    - CCDC (Cambridge Crystallographic Data Centre)
    - Hartree Centre, SFTC (Science and Technology Facilities Council, UK)
    - Pixact (Markus Honkanen)
  - Other partners in areas below
    - Secondary nucleation
    - Agglomeration kernel
    - Breakage kernel